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ABSTRACT: We have advanced the theory of localized defects on DNA homopolymer chains. This includes constructing operative computer code for the necessary numerical analysis. We have also developed the theory of atomic interactions and normal mode vibrational analysis on homopolymer DNA, working to give a strong physical basis to the numerical analysis. Some new phenomena have been predicted.

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Final Report: Storing Bits on a DNA Polymer Chain

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July 7, 1991

ABSTRACT: We have advanced the theory of localized defects on DNA homopolymer chains. This includes constructing operative computer code for the necessary numerical analysis. We have also developed the theory of atomic interactions and normal mode vibrational analysis on homopolymer DNA, working to give a strong physical basis to the numerical analysis. Some new phenomena have been predicted.

At the time of the beginning of this contract, attention in DNA physics was centered on the reported anomalous resonant absorption of microwaves by uniform length strands of DNA in solution. This measurement by workers at Maryland was anomalous because our group had, a few years earlier, published a series of theory papers on low frequency sound in DNA, and the observations contradicted our results. Thus we thought it worthwhile that initially considerable effort should be spent in an attempt to reconcile the theory and experiments. The published results of that effort appeared as items [1], [3], [4], [5], [10] & [12] in the list of published papers under this contract. The resolution we achieved, however, was never entirely satisfactory. The experimental results remained anomalous, at least in some degree. These observations were never repeated, although several groups tried to do so. Current opinion is that the measurements were in error, and the theory is sound.

With the confidence that our basic understanding of the damping process was sound, the work of the contract continued on two fronts: 1) the development of a strong first-principles physical basis for all interactions in DNA, and 2) the specific development of efficient algorithms and techniques to exploit this basis for local mode problems.

Item [6] - and also the closely related item [18] - were part of the general interactions problem. The calculations of these two papers first probed the "intermediate range" of normal mode frequencies. They also first revealed that different values for the basic parameters were apparently necessary in different frequency regimes. To explain the experimental values for sound speeds revealed by inelastic neutron scattering, it was necessary to use a different dielectric constant than that which gave satisfactory Brillouin scattering results. We also discovered that the separation into distinct frequency domains was surprisingly sharp at the upper limit of the "intermediate" frequency range; this

was published as item [13].

This discrepancy between necessary values of the same parameter in two different experiments brought out attention to the general importance of electrodynamics in the normal mode problem. We discovered then that our earlier methods of treating long range forces, essentially charge-charge interactions, was quite unsatisfactory. When proper treatment of the electrodynamic behavior of the composite medium of DNA polymer and solvent was given, the discrepancy between the parameter values in different frequency regimes was resolved. This work appeared as items [8], [9] & [20]. In addition the novel phenomenon of the one dimensional plasmon was discovered and predicted. This was discussed in item [7].

A related issue having to do with novel sorts of excitations arose in connection with the possibility of soliton propagation along the DNA polymer chain. That the important excitations might be solitonic, rather than ordinary harmonic waves, had been raised in connection with the anomalous "resonances" "observed" by the Maryland group. This suggestion was answered decisively in the negative in item [2]. However, the general question of the existence of solitonic states remained. Items [14] and [15] showed that such excitations might be possible, but that they were subject to strong damping from thermal collisions by solvent molecules. These results led to some controversy, even within Purdue, and these questions were answered in item [19].

The effort to give a genuine physical basis to the parametrization of the interactions between the polymer atoms continues. Items [21] and [23] are an exploration of the applicability of one of the most widely used descriptions of the hydrogen bonding that serves - at least in part - to hold the polymer chain together in the double helical structure.

We regard it of paramount importance that theory should be able to describe and predict experiments, not merely tabulate them. Hence we continue to search for experimental connections between

our work and spectroscopy. Item [17] concerns a potential method for making many such connections; it is, however, disappointing in that the precision of current experiments is not yet sufficient to make use of the methodology it develops. By contrast, item [22] explores a strong temperature dependence of the spectrum which should serve to make several important correspondences between theory and experiment.

The local mode problem is the key to the application to possible bit storage and manipulation on the polymer. The recently published item [16] is the culmination of a long effort to develop a working algorithm for treating local mode analysis. While only a single publication, it describes a reliable way of obtaining the necessary vibrational behavior for studying the bit storage question, and represents a long and arduous theoretical task. We undertook this task because we believe that other approaches to this problem are of uncertain value.

We are applying this new methodology presently under the new contract to selected test local defects in a search for experimental features that would serve to verify its predictions. We believe that such cautious exploration, closely guided by experiments, is more useful than premature calculation of more elaborate effects that could in the end turn out to be only computational artifacts.

Refereed Publications

[1] Theory of the anomalous resonant absorption of DNA at microwave frequencies, (w/M.E. Davis). J. of Biomolecular Structure and Dyn. 3, 1045-1053 (1986).

[2] A theorem on Boussinesq solitons or why soliton formation sharpens resonant absorption and why this has nothing to do with real polymers. J. of Bio. Struc. & Dyn. 4, 309-317 (1986).

[3] Resonant microwave absorption by dissolved DNA, L.L. Van Zandt Phys. Rev. Letts. 57, 2085-2087 (1986).

[4] Why structured water causes sharp absorption by DNA at microwave frequencies, L.L. Van Zandt J. of Bio. Structure & Dyn. 4, 239 (1987).

[5] Microwave response of DNA in solution: Theory, (w/M.E. Davis), Phys. Rev. A 37, 888 (1988).

[6] Helical lattice vibrational modes in DNA, (w/V.V. Prabhu/W.K. Schroll/ E. Prohofsky). Phys. Rev. Letters. 60, 1587-1588 (1988).

[7] DNA Plasmon, (w/V.K. Saxena). Phys. Rev. Letts. 61, 1788-1790 (1988).

[8] Effective field approach for long-range dissolved DNA polymer dynamics, (w/V.K. Saxena/W.K. Schroll). Phys. Rev. A39, 1474-1481 (1989).

[9] Millimeter-microwave spectrum of DNA: six predictions for spectroscopy, (w/V.K. Saxena). Phys. Rev. A39, 2672 (1989).

[10] Response of DNA in Aqueous solution to microwave irradiation, (w/M.E. Davis). Book of Abstracts Fifth Conversation in Biomolecular Stereodynamics June 2-6, 1987, pg. 316, ed. R.H. Sarma.

[11] Longitudinal phonon interpretation of inelastic neutron scattering in DNA, (w/W. Schroll). Biopolymers 28, 1189 (1989).

[12] Temperature and concentration behavior of anomalous microwave resonances in DNA, (w/M. Davis). Biopolymers 28, 1429 (1989).

[13] Atomic motions and high frequency cut-off in biological macromolecules, Chem. Phys. Lett. 164, 82 (1989).

[14] DNA solitons with realistic parameters values, Phys. Rev. A.40, Rapid Communications, 6134 (1989).

[15] Propagation of energy packets along model DNA polymer, L.L. Van Zandt, Book of Abstracts Sixth Conversation in Biomolecular Stereodynamics, Ed. R.H. Sarma, SUNY Albany, June (1989).

[16] Closed form solution for localized modes on a polymer chain with a defect, J. Comp. Phys. 93, 273 (1991).

[17] Determination of eigenvectors in molecular spectroscopy by isotopic substitution, Biopolymers 30, 87 (1990).

[18] Phonon Interpretation of Inelastic Neutron Scattering in DNA Crystals, W.K. Schroll, V.V. Prabhu, E.W. Prohofsky, and L.L. Van Zandt, Biopolymers 28, 1189-1193, (1989).

[19] Reply to `Comment on `DNA Solitons With Realistic Parameters'', L.L. Van Zandt, Phys Rev A 42, 5036-5039 (1990).

[20] Dynamics of Dissolved DNA Polymers Using a Frequency-Dependent

Dielectric Constant, V.K. Saxena and L.L. Van Zandt, Phys Rev A 42, 4993-4997, (1990).

[21] Modeling Hydrogen Bonds in Three Dimensions, L.L. Van Zandt and W.K. Schroll, J. of Bio. Struct. & Dyn. 8, 431-438 (1990).

[22] Identifying and Interpreting Spectral Features of Dissolved Poly(dA)-Poly(dT) DNA Polymer in High-Microwave Range, Phys Rev A 43, 4510-4516 (1991).

[23] Low-Frequency Parametrization of Hydrogen Bonding, W.K. Schroll, L.L. Van Zandt, and V.K. Saxena, J. of Bio. Struct. & Dyn. 8, 1057-1067, (1991).

Ph. D. Theses

Malcolm E. Davis, "Theory of the Response by DNA in Solution to Microwave ILlumination", Purdue University, April 1987.

Wayne K. Schroll, "Selected Topics on the Dynamics of DNA", Purdue University, Decenber 1990.

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